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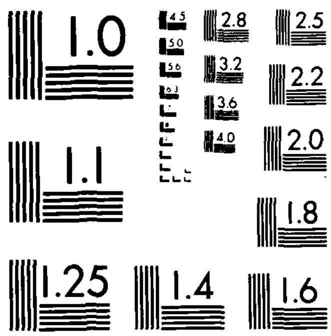

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A recursion exists among the coefficients of the color polynomials of some of the families of graphs considered in recent work of Balasubramanian and Ramaraj[1]. Such families of graphs have been called Fibonacci graphs. Application to king patterns of lattices is given. The method described here applies only to the so called Fibonacci graphs.

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On Color Polynomials of Fibonacci Graphs

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Abstract

A recursion exists among the coefficients of the color polynomials of some of the families of graphs considered in recent work of Balasubramanian and Ramaraj[1]. Such families of graphs have been called Fibonacci graphs. Application to king patterns of lattices is given. The method described here applies only to the so called Fibonacci graphs.

Key words

Graph Theory

Fibonacci Graphs

Color Polynomials

King Polynomial Graphs

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1. Introduction

Recently Balasubramanian and Ramaraj[1] wrote an interesting paper on a newly defined color polynomial of certain graphs. They related their work to the pioneering work of Motoyama and Hosoya[2] on king polynomials. Their paper has its merits in both the areas of statistical mechanics and "chemical" graph theory.

The purpose of this communication is to cite an observation on a recursive relation occurring amont the coefficients of the color polynomials of some of the families of graphs and their corresponding king patterns which they considered. The observation may be of value from both the computational and graph-theoretical viewpoints. The method which will be described here applies only to the so called Fibonacci graphs.[3]

2. Definition of Fibonacci Graphs[3]

In a homologous series of graphs the set $\{G_n, G_{n+1}, G_{n+2}, \dots\}$ where the number of vertices, n, may or may not be finite, has been called a set of Fibonacci graphs[3] if the following recursion is satisfied:

$$\theta(G_{n+2}, k+1) = \theta(G_{n+1}, k+1) + \theta(G_n, k) \tag{1}$$

where $\theta(G,k)$ is some graph-theoretical invariant of G which may include the following:

i) The number of k-matchings[4] in a graph

ii) The number of k mutually resonant but nonadjacent sextets when G=B, a benzenoid system

iii) The number of k independent sets of vertices when G=C, the so called Clar graph[5,6].

Inter-relations among these invariants have been recently published[7]. Hosoya[8] seems to be the first who observed recursive relations of the type of eqn. 1 but only for the paths and the cycles when $\theta(G,k)$ becomes the number of matchings and G is either a path or a cycle. Recently this author[3] and Gutman[9] generlized the concept to other types of graphS which obey eqn. (1) and to several graph invariants.

3. Construction of Fibonacci Graphs

The (finite or infinite) set $\{G_n, G_{n+1}, \ldots G_{n+s}\}$, $n \geq 0$, $s > n+1$ is called a set of Fibonacci graphs. Further, if either v_0 or v_1 is of degree one, then also $\{ G_{-1}, G_0, \ldots, G_n \}$ is a set of Fibonacci graphs. Such a set must possess at least three elements. The above construction is illustrated in Fig. 1 on the molecular graph of the benzyl radical. There are two modes of graph growth leading to Fibonacci graphs, i.e. "Fibonacci growth", viz., (a) external graph growth (path growth) and (b) internal graph growth (cycle growth).

4. Application to Color Polynomials[1] and king Patterns[1,2]

First we observe that the color polynomials given in ref. 1 are equivalent to the independence polynomials[5,6] introduced earlier. Thus $0(G,k)$ is defined[5,6] to be the number of selections of k independent vertices from G. This is precisely the number of ways of coloring k vertices black so that no two black vertices are adjacent. Table VII of ref. 1 lists color polynomials of some cycles. Of course a homologous series of rings form a set of Fibonacci graphs and thus should conform to eqn. 1 where $I(G,k) = 0(C;k)$, C = cycle*. The coefficients (i.e. $0(C;k)$'s)

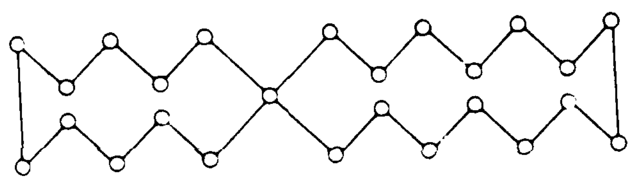
---

*Balasubramanian and Ramaraj[1] have shown that the coefficients of the color polynomials of the paths are the Fibonacci numbers while those of the cycles are manage numbers.

are reproduced here to demonstrate the validity of eqn. 1.

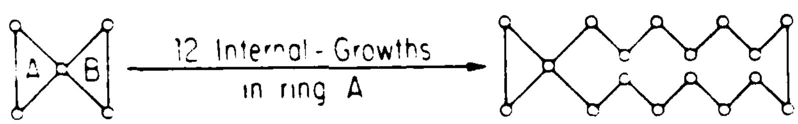
n					
2	1	2	0		
3	1	3	0		
4	1	4	2	0	
5	1	5	5	0	
6	1	6	9	2	0
7	1	7	14	7	0

As a further application of the concept of Fibonacci graphs we calculate the color polynomial of $G_{10,14}$; a graph on 25 vertices.



$G_{10,14}$

There are a number of routes for the homologation to $G_{10,14}$ from smaller graphs. One such route is indicated below



$G_{2,2}$ $G_{10,14}$

$$G_{2,14} \xrightarrow[\text{in ring B}]{\text{8 Internal - Growths}} G_{10,14}$$

Homologation to $G_{2,14}$ is shown in Table 1. To obtain $G_{10,14}$ from $G_{2,14}$ we need the color polynomial of $G_{3,14}$ which is calculated using recursion 2[7]

$$C(G;x) = C(G-v;x) + xC(G\theta\, v;v) \qquad (2)$$

where C(G;x) is the cycle polynomial[1,6,7] of Gand other symbols have their usual meanings. If one chooses the tetravalent vertex the polynomial is obtained in terms of (the known) path polynomials:

$$C(G_{3,14};x) = 1 + 18X + 134X^2 + 535X^3 + 1243X^4 + 1708X^5$$
$$1352X^6 + 575X^7 + 115X^8 + 8x^9$$

Then $G_{2,14}$ and $G_{2,15}$ are the first two leading Fibonacci graphs for the second internal growth in ring B (Table 2).

Obviously $G_{10,14}$ corresponds to the lattice in Fig. 2.

5. Conclusion

Recursive relations of form 1 are very helpful in construction of counting polynomials of potentially very large graphs. Such a buildup from very small units is conceptually similar to expanding the secular determinant of a graph by pruning it down to smaller fragments[10]. The identification of a particular family of a Fibonacci graph is certainly of topological and computational importance and is probably equivalent to a botanical identification of a plant family.

Acknowledgments

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References

1. K. Balasubramanian and R. Ramaraj, J. Comput. Chem. 6, 447 (1985).
2. A. Motoyama and H. Hosoya, J. Math. Phys. 18, 1485 (1985).
3. S. El-Basil, Theoret. Chim. Acta 65, 191 (1984), 65, 199 (1984).
4. H. Hosoya, Bull. Chem. Soc. Japan, 44, 2332 (1971).
5. I. Gutman, Z. Naturforsch 37a, 69 (1982).
6. I. Gutman and S. El-Basil, Z. Naturforsch 39a, 276 (1984).
7. S. El-Basil, J. Chem. Soc., Faraday Trans. 2, 82, 299 (1986).
8. H. Hosoya, The Fibonacci Quarterly, 14, 173 (1976).
9. I. Gutman and S. El-Basil, Math. Chem. in press.
10. K. Balasubramanian and M. Randić, Theoret. Chim. Acta, 61, 307 (1982).

Fig. Legends

Fig 1

The two types of Fibonacci growths of graphs:

(a) External subdivision and (b) Internal subdivision.

Fig. 2

The lattice graph corresponding to $G_{10,14}$. There are 34362 king patterns generated when 6 kings assume nontaking positions. (c.f. Tables 1 and 2). Observe that $G_{10,14}$ is the dualist graph of the above lattice.

Table 1

Homologation from $G_{2,2}$ to $G_{2,14}$. Numbers are coefficients of color polynomials. Relation 1 is observed throughout. The computation involves 12 "Fibonacci-growths".

1	5	4	0						
1	6	8	2	0					
1	7	13	6	0					
1	8	19	14	2	0				
1	9	26	27	8	0				
1	10	34	46	22	2	0			
1	11	43	72	49	10	0			
1	12	53	106	95	32	2	0		
1	13	64	149	167	81	12	0		
1	14	76	202	273	176	44	2	0	
1	15	89	266	422	343	125	14	0	
1	16	103	342	624	616	301	58	2	0
1	17	118	431	890	1038	644	183	16	0

Table 2

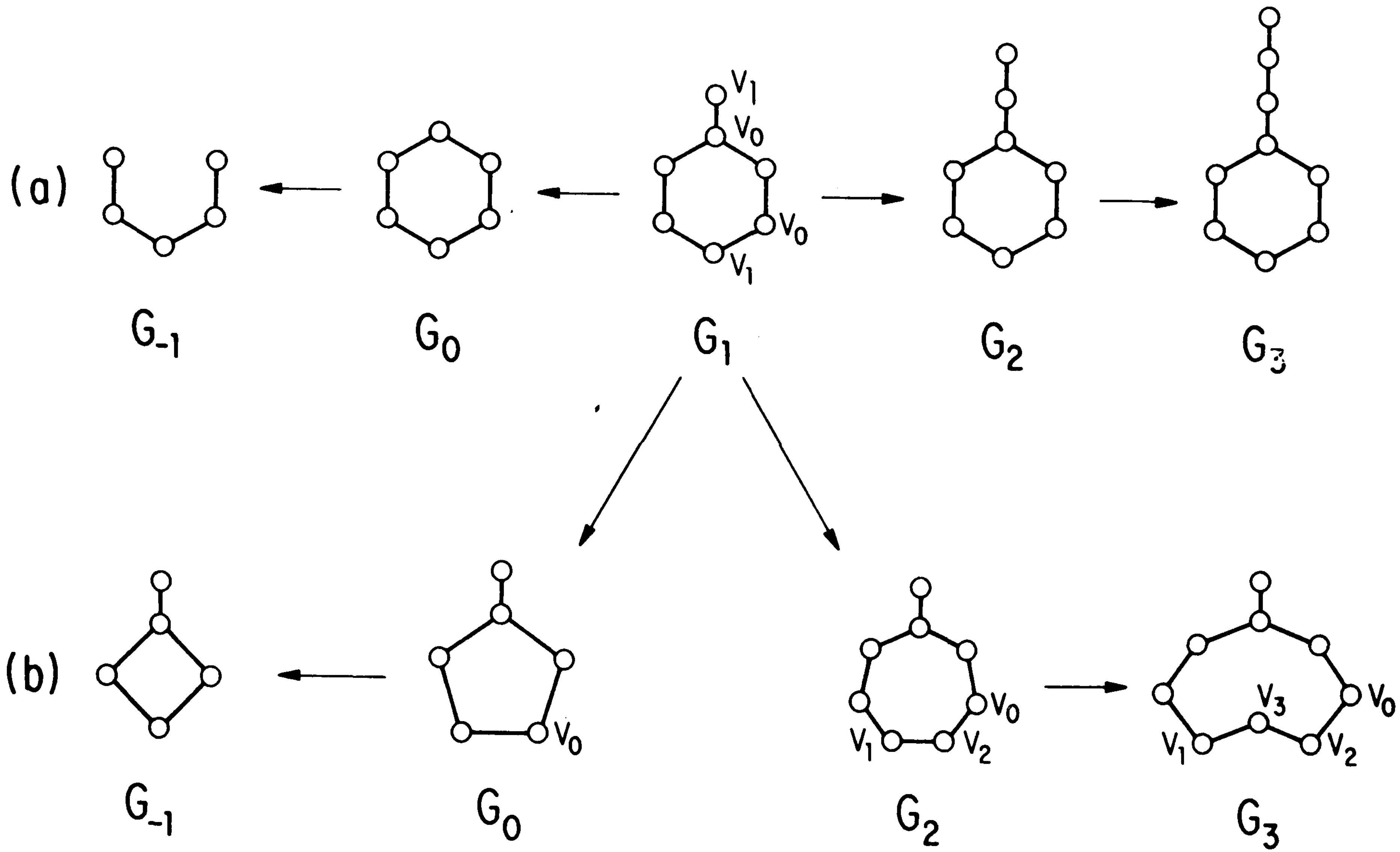
Homolgation $G_{2,14} \rightarrow G_{10,14}$ via 8 internal Fibonacci growths. Numbers are coefficients of color polynomials.

1	17	118	431	890	1038	644	183	16	0	
1	18	134	535	1243	1708	1352	575	115	8	0
1	19	151	653	1674	2598	2390	1219	298	24	0

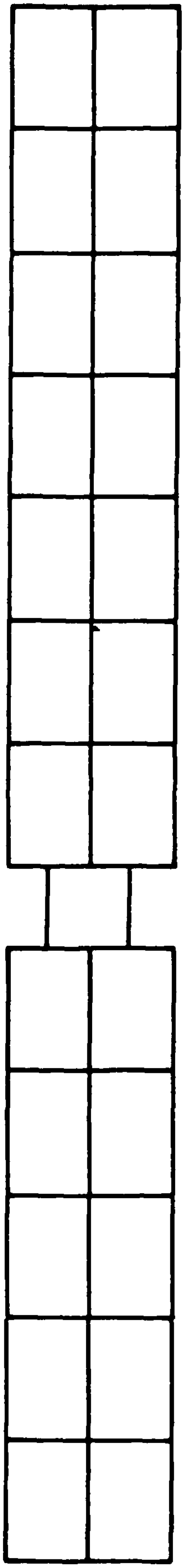
$\Downarrow$

1, 25, 274, 1732, 6989, 18822, 34362, 42344,

34438, 17689, 5320, 819, 48, 0.


(a)
G_{-1}
G_0
G_1
v_1
v_0
v_0
v_1
G_2
G_3
(b)
G_{-1}
G_0
v_0
G_2
v_0
v_1
v_2
G_3
v_3
v_0
v_1
v_2

Fig



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